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The Crystal Structure of Mercury(II) Acetamide

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Mercury(II) acetamide crystallizes in the monoclinic system, the space group $P2_1/c$, with two molecules per unit cell. The unit cell dimensions are: $a = 8.77 \pm 0.02$ Å, $b = 4.80 \pm 0.01$ Å, $c = 8.46 \pm 0.02$ Å, $\beta = 96.5 \pm 0.2°$, the measured and calculated densities are 2.95 and 2.97 g/cm³, respectively. The structure has been solved using 456 independent reflections collected about the a, b and c axes on integrated equi-inclination Weissenberg photographs and refined by least-square method to $R = 0.134$. The structure is built up of the discrete planar centrosymmetric $Hg(CH_3CONH)_2$ molecules containing two collinear covalent Hg–N bonds of 2.06 ± 0.06 Å. The oxygen atoms are 3.17 ± 0.06 Å from the mercury atom and the carboxyl-amide groups are not chelating groups in this structure. There are two oxygen atoms from two neighbouring molecules distant 2.88 ± 0.06 Å from the mercury atom. The molecules are linked together along the c axis by O–H...N hydrogen bonds of 3.05 ± 0.06 Å. The other bond lengths are within the range expected for this class of compounds.

Introduction

Covalently bonded mercury in mercury(II) acetamide has been anticipated due to the absence of typical reaction for mercury(II) ions in aqueous solutions.[1] There has been no direct evidence whether the co-ordinating bonds are to the nitrogen or oxygen atoms, but experience with amides in organic chemistry has produced the commonly accepted belief that in all metal carboxyl-amides the metal is bound to nitrogen. The decision is difficult because amides are very weak acids and the proton can be attached either to oxygen or to nitrogen.[2] For the substitution of proton by metal ion the nature of the metal could be decisive as well. It has also been suggested that both the nitrogen and oxygen atoms are bound to the metal atoms, as in the case of mercury(II) acetamide,[3,4] giving a chelate complex in which mercury would be in planar fourfold co-ordination. Such a structure is not likely to occur according to the known stereochemistry of mercury.[5] In addition there is no known structure of a mercury oxo-acid salt in which the anion has a symmetric function. This investigation was undertaken in order to investigate the crystal chemistry of mercury as well as to elucidate the bonding in a metal carboxyl-amide. It is interesting that neither the structure of this nor of any other metal carboxyl-amide has been determined so far.

(1) H. Ley and H. Kissel, *Ber. Dtsch. Chem. Ges.*, *32*, 1358 (1899).
(2) J. D. Roberts and M. C. Caserio, "Basic Principles of Organic Chemistry", W. A. Benjamin, Inc., New York, 1965, p. 680.
(3) L. Kahovec and K. Knollmüller, *Z. Physikal. Chem.*, *B*, *51*, 49 (1941).
(4) W. Kutzelnigg and R. Mecke, *Spectrochim. Acta.*, *18*, 549 (1962).
(5) D. Grdenić, *Quart. Rev. Chem. Soc., Lond.*, *19*, 303 (1965).

Experimental Section

Preparation and crystal data. Mercury(II) acetamide, $Hg(CH_3CONH)_2$, was prepared by dissolving mercury(II) oxide in the molten acetamide. The crystals from aqueous solution were obtained in the form of a crystalline mass and the separation of individual single crystals suitable for measurements was quite difficult.

The lattice parameters were determined from oscillation and Weissenberg photographs. The systematic absence of reflections $h0l$ for l odd and $0k0$ for k odd uniquely determined the space group as $P2_1/c$. Crystals data are collected in Table I.

Table I. Crystallographic data for $Hg(CH_3CONH)_2$.

M.W. = 316.67	
Crystallographic system: monoclinic	
Space group: $P2_1/c$ - C^5_{2h}	
Unit cell parameters:	$a = 8.77 \pm 0.02$ Å
	$b = 4.80 \pm 0.01$ Å
	$c = 8.46 \pm 0.02$ Å
	$\beta = 96.5 \pm 0.2°$
	$V = 353.8$ Å³
	$Z = 2$
$d_{calc} = 2.97$ g cm^{-3}	
$d_{obs} = 2.95$ g. cm^{-3} (picnometrically)	
$\mu_{CuK\alpha} = 426$ cm^{-1}	

Except for some weak reflections, all hkl reflections fulfil the condition of $k + l = 2n$ indicating the special position of the mercury atom. Three-dimensional X-ray diffraction intensity data ($hk0 \rightarrow hk7$, $h0l \rightarrow h4l$, and $0kl \rightarrow 5kl$) were taken on Nonius-Delft integrated equi-inclination Weissenberg photographs (multiple-film technique) using nickel-filtered copper K radiation. For the structure analysis 456 independent intensities were determined by means of a microdensitometer. After corrections for Lorenz and polarization factors the intensities were placed on the same relative scale. No absorption correction was used. The size of the crystal was $0.16 \times 0.13 \times \times 0.06$ mm.

Table II. Observed and calculated structure factors. The values listed are $50F_o$ and $50F_c$.

h	k	l	F_o	F_c
0	0	2	7754	7954
		4	6064	5138
		6	4965	4209
		8	2887	2695
		10	1435	1854
0	1	1	5499	5107
		2	1874	-1393
		3	6779	5657
		4	797	-381
		5	5523	4299
		7	3555	3653
		9	2301	2392
0	2	0	6598	6744
		2	7276	5867
		4	6451	5061
		6	4542	3468
		8	2162	2129
		10	1059	1623
0	3	1	3948	3766
		3	5465	4087
		5	3985	2895
		7	2193	2217
		9	1356	1694
0	4	0	3632	3277
		2	3437	2937
		4	3189	2707
		6	2256	2206
		8	891	1443
0	5	1	2138	2187
		3	1967	1812
		5	1154	1426
0	6	0	860	1397
		2	700	1263
1	0	-10	1622	2068
		-8	3653	3461
		-6	4559	4774
		-4	5994	6234
		-2	5633	6157
		0	3758	8357
		2	8104	8890
		4	4402	4320
		6	3469	3290
		8	2589	2531
		10	929	1490
1	1	-9	1830	2053
		-7	3015	3282
		-5	5377	4472
		-4	1352	-769
		-3	5785	4947
		-2	1068	666
		-1	7180	7423
		0	1035	988
		1	5945	6404
		2	1080	-666
		3	6819	5566
		4	892	-604
		5	6013	4801
		7	3233	3287
		9	2200	2371
1	2	-10	1188	1819
		-8	2950	2744
		-6	4578	3441
		-4	6930	5385
		-2	7229	6263
		0	4359	5305
		2	6268	5265
		4	5327	3972
		6	3759	3040
		8	2013	2036
		10	696	1309
1	3	-9	1301	1709
		-7	2099	2301
		-5	3820	2855
		-3	4614	3554
		-1	4549	4363
		1	3960	3843
		3	5206	3993
		5	4594	3501
		7	1952	2113
		9	1006	1480
1	4	-8	955	1556
		-6	2104	2125
		-4	3302	2959
		-2	3543	3213
		0	2554	3045
		2	2989	2801
		4	2358	2130
		6	1859	1841
		8	726	1417
1	5	-5	1123	1590
		-3	1476	1616
1	5	-1	1811	2019
		1	2056	2202
		3	1794	1937
		5	1224	1521
1	6	-2	420	1274
		-1	829	187
		0	811	1336
		1	766	200
		2	508	1267
2	0	-10	1604	2036
		-8	3326	3274
		-6	5026	5108
		-4	5463	5675
		-2	4884	5399
		0	2631	4317
		2	5143	5441
		4	5042	4918
		6	3329	3007
		8	2396	2471
		10	1210	1603
2	1	-9	1949	2332
		-7	2600	2960
		-5	5681	4721
		-4	1460	-903
		-3	6828	6120
		-2	1086	-990
		-1	5518	7004
		0	971	971
		1	6997	8618
		3	6239	5747
		5	4480	3913
		7	2457	2826
		9	1427	1752
2	2	-10	1110	1826
		-8	2981	2844
		-6	4798	3626
		-4	5116	4024
		-2	5894	5682
		0	3767	4686
		2	4074	3614
		4	4663	3802
		6	3332	2779
		8	1850	1997
2	3	-9	1268	1810
		-7	2049	2338
		-5	3930	3131
		-3	4936	3961
		-1	4391	4334
		1	4242	4253
		3	4303	3413
		5	3956	3066
		7	1825	2172
		9	701	1176
2	4	-8	924	1588
		-6	2004	2064
		-4	2555	2421
		-2	3060	2999
		0	2439	2925
		2	2422	2569
		4	2157	2139
		6	1505	1508
2	5	-5	1336	1780
		-3	1666	1852
		-1	1596	1770
		1	1761	2022
		3	1539	1823
		5	1033	1418
2	6	0	622	1256
3	0	-10	1690	2133
		-8	2254	2514
		-6	4090	3949
		-4	5673	5631
		-2	3835	4865
		0	3703	5058
		2	4355	4704
		4	4451	4303
		6	3465	3347
		8	2037	2130
		10	856	1523
3	1	-9	2232	2523
		-7	3222	3648
		-5	5123	4516
		-3	6454	6367
		-2	1309	-954
		-1	4842	6251
		1	4742	5802
		3	5509	5429
		5	3221	3005
		7	1635	2058
		9	1250	1444
3	2	-10	986	1825
		-8	2355	2469
		-6	4163	3307
		-4	4317	3665
		-2	4103	4033
		0	4388	5180
		2	3714	3836
		4	3709	3254
		6	3086	2927
		8	1661	1818
3	3	-9	1139	1748
		-7	2308	2607
		-5	3738	3038
		-3	4663	3979
		-1	4272	4347
		1	3714	3595
		3	3353	2881
		5	2656	2161
		7	1389	1769
3	4	-8	958	1542
		-6	1828	1978
		-4	2169	2238
		-2	2160	2333
		0	2505	2731
		2	2246	2535
		4	2016	2113
		6	1237	1580
3	5	-5	1163	1659
		-3	1738	2020
		-1	1476	1825
		1	1404	1642
		3	1248	1590
		5	725	1174
4	0	-10	1604	2019
		-8	2455	2630
		-6	2854	2860
		-4	4964	4893
		-2	5348	6295
		0	4258	5246
		2	4844	5429
		4	4067	3956
		6	2691	2627
		8	1669	1755
4	1	-9	2201	2434
		-7	3226	3534
		-5	4992	4596
		-3	4461	4636
		-1	3923	4946
		1	3236	3721
		3	3626	3359
		5	3273	3039
		7	1446	1787
		9	902	1247
4	2	-8	2300	2401
		-6	3352	2950
		-4	3996	3697
		-2	3685	4160
		0	4206	4548
		2	4374	4497
		4	3098	2921
		6	2272	2245
		8	1399	1645
4	3	-9	1022	1670
		-7	2149	2435
		-5	3586	2983
		-3	3297	2942
		-1	3475	3614
		1	3384	3225
		3	2372	2230
		5	1945	1794
		7	1004	1331
4	4	-6	1520	1876
		-4	2200	2296
		-2	2169	2357
		0	2081	2219
		2	2399	2316
		4	1796	1899
		6	1056	1430
4	5	-5	925	1437
		-3	1402	1717
		-1	1463	1786
		1	1223	1485
		3	1014	1281
5	0	-10	1673	1940
		-8	2972	2784
		-6	3551	3394
		-4	3898	3815
		-2	5108	5654
		0	4627	5186
		2	3925	3829
		4	3750	3456
		6	2111	1992
5	0	8	1123	1140
5	1	-9	2161	2287
		-7	2441	2733
		-5	4013	3579
		-3	4114	4125
		-1	3039	3518
		1	3139	3436
		3	2844	2679
		5	2771	2393
		7	1551	1924
5	2	-8	2166	2202
		-6	3260	3180
		-4	3497	3473
		-2	3833	3973
		0	3917	3972
		2	3724	3421
		4	2764	2623
		6	1678	1533
		8	929	1137
5	3	-7	1625	2038
		-5	2931	2558
		-3	2713	2512
		-1	2512	2349
		1	3006	2882
		3	2266	2266
		5	1694	1549
		7	1086	1225
5	4	-6	1531	1841
		-4	2046	2130
		-2	2335	2409
		0	2111	2113
		2	1739	1684
		4	1518	1500
		6	646	1076
5	5	-3	1225	1406
		-1	1164	1444
		1	1233	1363
		3	806	1136
6	0	-8	3046	2649
		-6	3781	3395
		-4	3886	3687
		-2	3754	3562
		0	3947	3810
		2	2820	2976
		4	2561	2019
		6	1876	1837
		8	728	951
6	1	-9	1665	1867
		-7	1959	2450
		-5	2897	2559
		-3	3707	3447
		-1	3661	3335
		1	3067	3180
		3	2885	2824
		5	2020	1930
		7	1065	1414
6	2	-8	1987	1998
		-6	3029	2760
		-4	3470	3371
		-2	2930	2901
		0	2946	2903
		2	2541	2467
		4	2040	1802
		6	1297	1314
6	3	-7	1285	1846
		-5	2290	2142
		-3	2413	2399
		-1	2291	2159
		1	2208	2095
		3	1942	2205
		5	1312	1469
6	4	-6	1094	1538
		-4	1658	1851
		-2	1620	1903
		0	1626	1905
		2	1283	1432
		4	1024	1013
6	5	-1	725	1249
		1	762	1087
7	0	-8	2686	2260
		-6	3189	2643
		-4	3391	2868
		-2	3161	2828
		0	2695	2373
		2	2398	2104
		4	1698	1410
		6	1447	1297
7	1	-7	1727	2200
		-5	3048	2665
		-3	2838	2640
		-1	3481	3311
7	1	1	3106	3036
		3	2103	2145
		5	1596	1627
		7	704	915
7	2	-8	1665	1847
		-6	2114	2033
		-4	2811	2536
		-2	2504	2484
		0	2026	1805
		2	2042	1896
		4	1510	1492
		6	924	1032
7	3	-7	977	1513
		-5	2161	2037
		-3	2195	2179
		-1	2124	2122
		1	1839	1730
		3	1185	1478
		5	835	1235
7	4	-4	1178	1377
		-2	1279	1442
		0	1167	1354
		2	996	1291
		4	437	910
8	0	-8	1886	1564
		-6	2394	2093
		-4	2355	2011
		-2	2650	2232
		0	2708	2333
		2	1949	1812
		4	1413	1394
		6	923	910
8	1	-7	1551	1985
		-5	2695	2400
		-3	2579	2458
		-1	2203	2038
		1	2376	2119
		3	1652	1554
		5	1021	1008
8	2	-6	1697	1688
		-4	1836	1727
		-2	2140	2042
		0	1795	1715
		2	1409	1354
		4	1109	1361
8	3	-5	1583	1571
		-3	1888	1909
		-1	1707	1674
		1	1338	1395
		3	914	1015
8	4	-2	791	1105
		0	751	1054
		2	531	931
9	0	-6	1497	1587
		-4	2104	1090
		-2	1835	1629
		0	2333	1903
		2	1738	1765
		4	1052	1109
9	1	-7	1018	1669
		-5	1859	1794
		-3	1979	1840
		-1	1600	1560
		1	1313	1107
		3	1213	1084
		5	584	741
9	2	-6	997	1344
		-4	1410	1556
		-2	1428	1559
		0	1575	1621
		2	1000	1230
		4	677	885
9	3	-3	1367	1252
		-1	1197	1294
		1	842	943
		3	250	783
10	0	-4	1511	1574
		-2	1425	1489
		0	1251	1068
		2	1188	1165
10	1	-5	1075	1322
		-3	1184	1233
		-1	1159	1224
		1	932	1016
		3	685	717
10	2	-4	813	1227
		-2	995	1307
		0	871	1098
		2	555	925
11	0	-2	904	1096
		0	692	772
11	1	-1	587	890

Table III. Co-ordinate and thermal parameters [a] with their estimated standard deviations [b].

Atom	x/a	y/b	z/c	B(Å²)
Hg	0.000	0.000	0.000	—
N	0.149(7)	−0.192(16)	−0.136(7)	3.72(1.2)
O	0.210(5)	−0.538(13)	0.040(5)	3.29(0.8)
C	0.235(8)	−0.383(17)	−0.085(9)	3.26(1.3)
$C(CH_3)$	0.350(7)	−0.534(20)	−0.188(7)	3.41(1.2)

	b_{11}	b_{22}	b_{33}	b_{23}	b_{13}	b_{12}
Hg	0.0129(4)	0.0317(14)	0.0081(4)	−0.0010(104)	0.0075(7)	−0.0061(159)

[a] The anisotropic temperature factors for the Hg atom are in the form: $\exp[-(b_{11}h^2+b_{22}k^2+b_{33}l^2+b_{23}kl+b_{13}hl+b_{12}hk)]$. [b] Standard deviations are in parentheses in terms of the least significant digits of the parameters.

Structure Determination. The special position 2(*a*) of mercury was shown by two Patterson projections obtained by means of the von Eller photosommateur. A three-dimensional Fourier synthesis was calculated phased on the mercury atom position. The first Fourier synthesis showed all the light atoms. Five cycles of the least-squares refinement, with isotropic thermal parameters for all atoms, resulted in a reliability index of $R = 0.168$. Four cycles of the refinement process were computed using anisotropic thermal parameters for the mercury atom only. Unit weight was used for all observations. The final value of the reliability index is $R = 0.134$. Further refinement was not possible due to unfavourable spot shape and neglecting absorption. The maximum shift in the final cycle of least-squares was less than 0.1σ. The observed and calculated structure factors are given in Table II. The final positional and thermal parameters together with their estimated standard deviations are given in Table III. The F_c values were calculated using the atomic scattering factors of Thomas and Umeda for mercury,[6] of Berghuis, Haanapel, Potters, Loopstra, MacGillavry and Veenendaal for oxygen, nitrogen and carbon.[7]

Structure factors and the Fourier synthesis were calculated on the Ferranti Mercury computer at the University of Sheffield while the refinement procedure was performed on the Science Research Council Atlas computer at Didcot, England.

Results and Discussion

It is seen imediately from the data in Table IV as well as from Figure 1 that mercury(II) acetamide does not have a chelate structure.

One atom of the carboxyl-amide group is closely bound to the mercury atom at a distance of 2.06 Å. Whether this atom is the nitrogen or the oxygen atom cannot be established from the X-ray diffraction data owing to the small difference between the scattering power of carbon and oxygen. Nevertheless, the unambigous answer is obtained by analyzing the lengths of the adjacent bonds.

If the atom in question is denoted by *A*, then the bond length of Hg–*A* as determined permits both possibilities for *A*, the oxygen or the nitrogen atom, since the value of 2.06 Å corresponds to the Hg–O bond as found in the structure of mercury(II) oxide[9] or in mercury(II) oxonium compounds,[10] as well as to the Hg–N bond, as found in the structure of Millon's base[11] or in amidomercury(II) halides.[12] On the other hand, the bond C–*A*, which is found to be 1.23 Å, cannot be a C–O bond, because this value is too short for a single carbon-oxygen bond, for

Table IV. Intramolecular and intermolecular distances (in Å) and angles[a] (in deg.) with their estimated standard deviation[b,8]

Hg–N	2.06(6)	O^{iii}–H...N	3.05(6)
C –N	1.23(9)	O–CH_3^{ii}	3.70(6)
C –O	1.33(8)	CH_3–CH_3^{iv}	3.80(8)
C –CH_3	1.58(9)	N–C–O	123.3(1.6)
Hg–O	3.17(6)	N–C–CH_3	123.4(1.6)
Hg–O^i	2.88(6)	O–C–CH_3	110.6(1.2)
Hg–CH_3^{ii}	3.82(7)		

[a] The positions are denoted as follows: no label x, y, z; (i) x, 1+x, z; (ii) x, −1/2−y, 1/2+z; (iii) x, −1/2−y, −1/2+z; (iv) 1−x, −1/2+y, −1/2−z. [b] Standard deviations are given in parentheses.

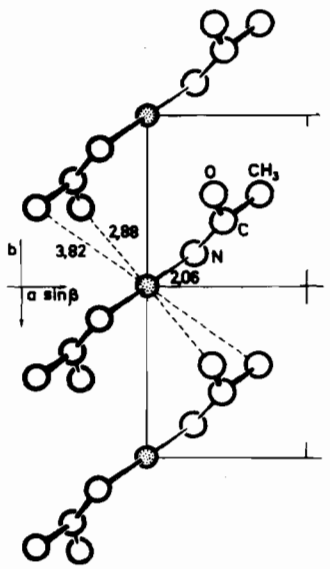
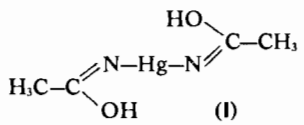


Figure 1. The arrangement of mercury(II) acetamide molecules projected down the *c*-axis. The oxygen-to-mercury and methyl-to-mercury approaches are shown by broken lines.

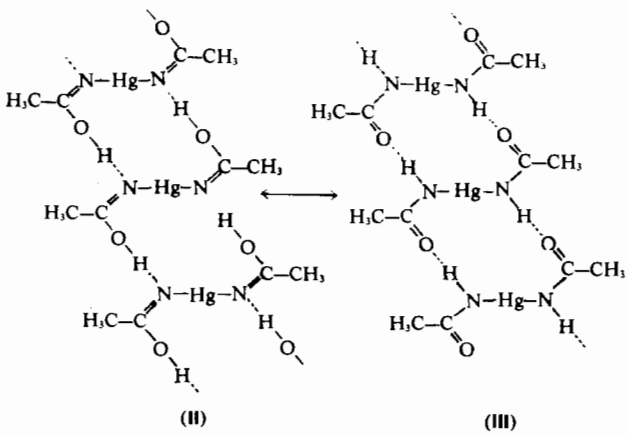
(6) L. H. Thomas and K. Umeda, *J. Chem. Phys.*, *26*, 293 (1957).
(7) J. Berghuis, I. J. M. Haanapel, M. Potters, B. O. Loopstra, C. H. MacGillavry, and A. L. Veenendaal, *Acta Cryst.*, *8*, 478 (1955).
(8) "International Tables for X-ray Crystallography", Vol. II, Kynoch Press, Birmingham, 1959, p. 331.
(9) K. Aurivillius, *Acta Chem. Scand.*, *18*, 1305 (1964).
(10) S. Ščavničar and D. Grdenić, *Acta Cryst.*, *8*, 275 (1955).
(11) W. N. Lipscomb, *Ann. N. Y. Acad. Sci.*, *65*, 427 (1957).
(12) (a)K. Brodersen and W. Rüdorff, *Z. Naturforsch.*, *9b*, 164 (1954); (b) K. Brodersen, *Acta Cryst.*, *8*, 723 (1955).

which a value of not less than 1.43 Å must be expected. Consequently, *A* is the nitrogen atom and the bond of 1.23 Å is a carbon-nitrogen double bond. The value agrees with the sum of the covalent double-bond radii as well as with the values found in the structure of bis(acetamidine)-platinum(II) chloride monohydrate[13] and in the structure of dimethylglyoxime.[14] Consequently, the nitrogen atom is covalently bound to mercury and the formula of mercury(II) acetamide is



(I)

The carbon-oxygen bond length of 1.33 Å, however, is considerably shorter than a single bond required by the above formula (I). It corresponds to the carbon-oxygen bond in carboxylic acids which approaches the double bond as, for instance, in acetic acid where it is 1.29 and 1.36 Å in the crystal structure and in the gaseous dimer respectively.[15] In the crystal structures of the acetamide the C–O bond is even shorter and amounts to 1.26 and 1.28 Å in the orthorombic and trigonal modification respectively.[16] It follows that the C–O bond in mercury(II) acetamide is not a single bond, as required by the formula (I) but is a partial double bond as in free carboxyl-amides or in carboxylic acids. The intermediate character of this bond in both latter classes of compounds is the result of resonance which increases as the carboxylic group becomes more symmetric. This can be achived by hydrogen bonding or by salt formation.[17] In mercury(II) acetamide this tendency cannot be fulfilled within the molecule, but can be by intermolecular interactions. Hydrogen bonding between the molecules allows resonance such as given by the formulae (II) and (III).



(II) (III)

Each molecule forms two O–H...N hydrogen bonds, one through the donating OH group, and one through the accepting N atom. They are equal in length, 3.05 Å, and they link the molecules in an endless puckered ribbon along the *c* axis (Figure 2). Due to resonance (II)↔(III) the protons in the hydrogen bonds occupy statistically two positions, near the oxygen atom and near the nitrogen atom, in the sense of Hunter's mesohydric tautomerism.[18] This explains the appearance of two NH-bands in the Raman[3] and in the IR spectra.[4] The absence of the C–O double-bond frequency in the spectra is also explained, since the proposed formula requires an intermediate single-double bond with bond length similar to that in acetic acid or in the free acetamide.

The tendency for hydrogen bonding, as required by the proposed structure, explains the high solubility in water as well as some properties of aqueous solutions observed by previous authors.[19]

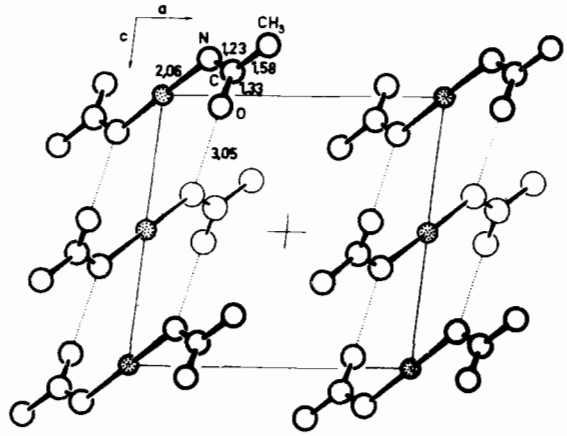


Figure 2. The structure of mercury(II) acetamide projected down the *b*-axis. The hydrogen bonds are shown by dotted lines.

The ribbons are arranged towards each other in such a way that the oxygen atoms of the adjacent molecules approach the mercury atom from both sides at a distance of 2.88 Å. This distance is equal to the sum of the van der Waals radii(1.50+1.40 Å).[5] The two oxygen atoms which belong to the same molecule are 3.17 Å apart from the mercury atom. This distance is larger than the sum of the van der Waals radii and cannot be included in the mercury co-ordination sphere. Two methyl groups from two neighbouring molecules complete the intermolecular approaches about the mercury atom at 3.82 Å.

The carbon-carbon bond length of 1.58 Å is similar to that found in bis(acetamide)cadmium(II) chloride.[20]

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(13) N. C. Stephenson, *J. Inorg. Nucl. Chem., 24,* 801 (1962).
(14) "Interatomic Distances", The Chemical Society, London, 1958, p. M 170.
(15) G. C. Pimentel and A. L. McClellan, "The Hydrogen Bond", W. H. Freeman and Company, San Francisco, 1960, p. 266.
(16) W. C. Hamilton, *Acta Cryst., 18,* 866 (1965).
(17) L. Pauling, "The Nature of the Chemical Bond", 3rd edn., Cornell University Press, Ithaca, 1960, p. 275.
(18) G. C. Pimentel and A. L. McClellan, "The Hydrogen Bond", W. H. Freeman and Company, San Francisco, 1960, p. 239.
(19) A. Weiss and Al. Weiss, XVIth International Congress of Pure and Applied Chemistry, Congress Handbook, Vol. 1, Paris, 1957, p. 118.
(20) L. Cavalca, M. Nardelli, and L. Coghi, *Nuovo Cimento, 6,* 278 (1957).